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Multiscale Simulation of Ionic Flux through a Nanopore under Applied Electric Potential BERT DEBUSSCHERE, HELGI ADALSTEINSON, BLAKE SIMMONS, KEVIN LONG, HABIB NAJM, Sandia National Laboratories — This talk discusses the development of an atomic/continuum multiscale model for the simulation of electrophoretically driven ionic fluxes through a nanopore of an electrodesalination membrane. The ion transport in this single pore model is simulated using Brownian Dynamics computations, with parameter fields that are obtained from targeted Molecular Dynamics simulations. The Brownian Dynamics simulations couple with a fine-grained Poisson-Nernst-Planck continuum model in the pore vicinity. The model is calibrated against patch clamp measurements of current through track-etched nanoporous membranes under an applied electric potential. Simulations are performed to investigate the effects of pore size, membrane wall charge and applied potential on the pore throughput and selectivity.

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